

Enhancing Problem Solving in Excel and MATLAB with Polymath 6.1*

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Outline

- Assessing the *computing needs* in undergraduate and graduate ChE education*
- Selecting *a set of software packages* to fulfill the computing needs
- Demonstration of the *advantages and disadvantages* of the various software packages by solving a benchmark problem.
- *Combining* the various software *packages* for more effective and efficient problem solving
- Conclusions

*See also Edgar, T. F., "Enhancing the Undergraduate Computing Experience", *Chem. Eng. Edu.*, 40 (3), 231(2006)

Assessing the computing needs in undergraduate and graduate ChE education

Ten Representative Problems from the ChE curriculum were prepared for the ASEE Chemical Engineering Summer School held in Snowbird, Utah on August 13, 1997.

The ten problems were solved using six software packages:

Excel - Edward M. Rosen

Maple - Ross Taylor

Mathematica - H. Eric Nuttall

Mathcad - John J. Hwalek, University of Maine

MATLAB - Joseph Brule, John Widmann, Tae Han, and Bruce Finlayson

POLYMATH - Michael B. Cutlip, and Mordechai Shacham

Assessing the computing needs in undergraduate and graduate ChE education

➤The ASEE summer school presentations identified advantages and disadvantages of the various software packages and lead to the conclusion (see: *Comput. Appl. Eng. Educ.* 6: 169-180, 1998) that there is a need to use a set of several packages in ChE education.

➤One possible set of packages with a CACHE* connection:

- POLYMATH* – Serves as a general, easy to use, user friendly *Problem Solving Environment* (PSE)

- Excel – Serves as a *spreadsheet based PSE* (the PSE most widely used by practicing engineers)

- MATLAB – Serves as a *programming language* and symbolic manipulation tool.

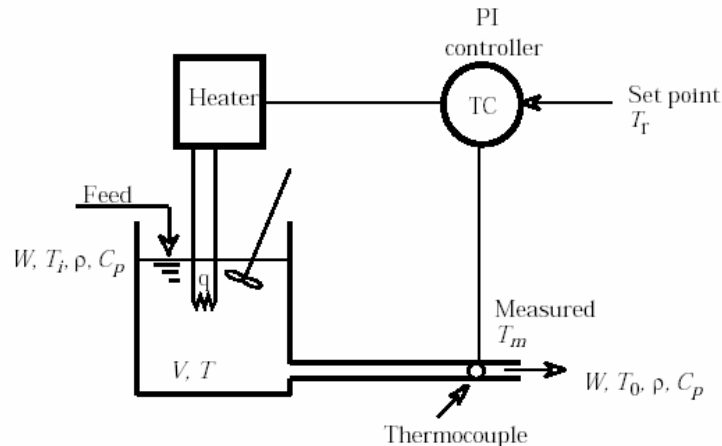
POLYMATH 6.1 Educational

- A proven computational system (PSE, Problem Solving Environment) that supports advanced problem solving in chemical, biochemical and other engineering disciplines.
- Capabilities include Linear Equations, Nonlinear Equations, Differential Equations, Data Analysis and Regression.
- Low-cost site licenses are provided through the CACHE Corporation for academic departments. These licenses enable use in computer labs and distribution of individual copies to all student, faculty, and staff.
- Individual use educational and professional versions are also available.
- POLYMATH has a *minimal learning curve* and provides *extensive error checking* during problem entry that leads to great efficiency in problem solution.

Limitations of the Individual Packages

- In POLYMATH, the easiness of use and user friendliness dictate a *fixed set of capabilities and options*. When a particular problem does not fit into the options provided, repeated manual rerunning of the problem may be necessary.
- In Excel, the PSE options were added in a late stage of development. Thus the *problem specification* (using cell addresses instead of variable names) *is difficult* and the documentation of the problem statement is hard to understand.
- In MATLAB (as in other programming languages), it is the user's responsibility to *take care of many technical details* of the solution that can be more efficiently done by the computer (like arranging the equations in the calculation order). The error messages may not be clear enough for a novice user.

DYNAMICS OF A HEATED TANK WITH PI TEMPERATURE CONTROL* (DHT) – An Example



*Problem No. 10 presented in the session of "The Use of Mathematical Software Packages in ChE" in the ASEE ChE Summer School, Snowbird, Utah, 1997.

DHT Example – POLYMATH MODEL

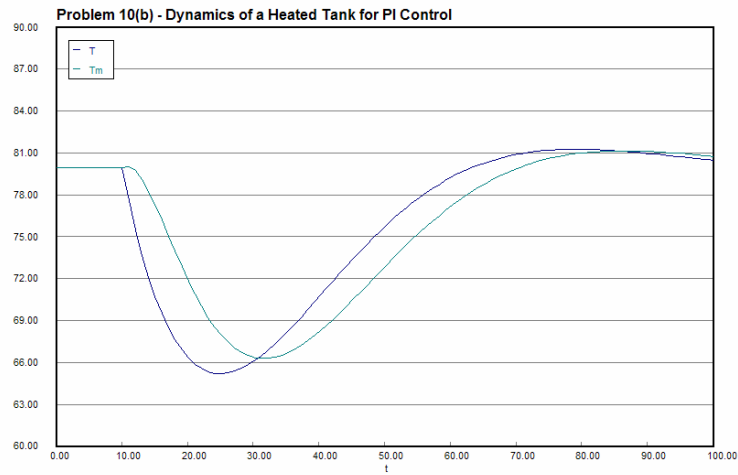
```

d(e)  x=  imi-  RKF45  Iable  Graph  Report
+  +  finl  i  i  i
Differential Equations: 4  Auxiliary Equations: 10  Ready for solution

#Problem 10 - Closed loop dynamics of a stirred tank heater
d(T)/d(t)=(WC*(Ti-T)+q)/rhoVCp # Temperature in the stirred tank (deg. C)
d(T0)/d(t)=(T-T0-(taud/2)*((WC*(Ti-T)+q)/rhoVCp))/taud # Time delayed temperature by f
d(Tm)/d(t)=(T0-Tm)/taum # Temp. measured by the thermocouple (deg. C)
d(errsum)/d(t)=Tr-Tm # Integral of the difference between set point and measured temps.

#The explicit equations
q=10000+Kc*(Tr-Tm)+Kc/taul*errsum # Heat supply (kJ/min)
Tr = 80 # Set point temperature (deg. C)
WC=500 # (Flow rate)*(heat capacity) (kJ/min-deg. C) # Initial values of the differential variables
rhoVCp=4000 # mass in tank*(heat capacity) (kJ/d T(0) = 80
Kc = 50 # Proportional gain of the PI controller (kJ/d T0(0)=80
taud=1 # Dead time (min) Tm(0) = 80
taum=5 # Thermocouple time constant (min) errsum(0) = 0
taul=2 # Reset time (min) # Initial/final values of the independent differ
Ti=60+step # Feed temperature (deg. C) t(0) = 0
step = if (t < 10) then (0) else (-20) # Step change in feed temperature (deg. C) t(f) = 100
    
```

DHT Example – POLYMATH SOLUTION



DHT Example – Excel SOLUTION

F7 $\text{=rk4}(\text{\$B\$15}, \text{\$E6}, \text{\$F6}, \text{\$G6}, \text{\$H6}, \text{\$I6}, 0.2, \text{\$B\$6})$

	A	B	C	D	E	F	G	H	I
1	Problem 10(b)								
2	Dynamics of a Heated Tank with PI Temperature Control								
3									
4	Parameters	Value	Index		Time (min)	T	To	Tm	errsum
5					0	80	80	80	0
6	rhoVCp - kJ/C	4000	0		0.5	80	80	80	0
7	Tis - C	60	1		1	80	80	80	0
8	taud - min	1	2		1.5	80	80	80	0
9	Kc - kJ/min-C	50	3		2	80	80	80	0
10	WCp - kJ/min-C	500	4		2.5	80	80	80	0
11	Tr - C	80	5		3	80	80	80	0
12	taum - min	5	6		3.5	80	80	80	0
13	taul - min	2	7		4	80	80	80	0
14			8		4.5	80	80	80	0
15	Integration Increment - h	0.5	9		5	80	80	80	0
16			10		5.5	80	80	80	0
17			11		6	80	80	80	0
18			12		6.5	80	80	80	0
19			13						

Note the use of cell addresses instead of variable names

The worksheet does not provide enough information regarding the model used. It cannot serve as stand alone documentation

Visual Basic Program for Fixed Step Size RK Integration by E. M. Rosen

```

'h = step size
'x = independent variable
'y1, y2, y3, y4, y5 = dependent variables

'nr = number of dependent variable to return =rk4
'prm a parameter vector of unspecified length
'kij : i is the k value, j is the equation number or dependent variable

k11 = fff1(x, y1, y2, y3, y4, y5, prm)
k12 = fff2(x, y1, y2, y3, y4, y5, prm)
k13 = fff3(x, y1, y2, y3, y4, y5, prm)
k14 = fff4(x, y1, y2, y3, y4, y5, prm)
k15 = fff5(x, y1, y2, y3, y4, y5, prm)

k21 = fff1(x + 0.5 * h, y1 + 0.5 * h * k11, y2 + 0.5 * h * k12, y3 + 0.5 * h * k13, y4 + 0.5 * h * k14, y5 + 0.5 * h * k15, prm)
k22 = fff2(x + 0.5 * h, y1 + 0.5 * h * k11, y2 + 0.5 * h * k12, y3 + 0.5 * h * k13, y4 + 0.5 * h * k14, y5 + 0.5 * h * k15, prm)
k23 = fff3(x + 0.5 * h, y1 + 0.5 * h * k11, y2 + 0.5 * h * k12, y3 + 0.5 * h * k13, y4 + 0.5 * h * k14, y5 + 0.5 * h * k15, prm)
k24 = fff4(x + 0.5 * h, y1 + 0.5 * h * k11, y2 + 0.5 * h * k12, y3 + 0.5 * h * k13, y4 + 0.5 * h * k14, y5 + 0.5 * h * k15, prm)
k25 = fff5(x + 0.5 * h, y1 + 0.5 * h * k11, y2 + 0.5 * h * k12, y3 + 0.5 * h * k13, y4 + 0.5 * h * k14, y5 + 0.5 * h * k15, prm)

k31 = fff1(x + 0.5 * h, y1 + 0.5 * h * k21, y2 + 0.5 * h * k22, y3 + 0.5 * h * k23, y4 + 0.5 * h * k24, y5 + 0.5 * h * k25, prm)
k32 = fff2(x + 0.5 * h, y1 + 0.5 * h * k21, y2 + 0.5 * h * k22, y3 + 0.5 * h * k23, y4 + 0.5 * h * k24, y5 + 0.5 * h * k25, prm)
k33 = fff3(x + 0.5 * h, y1 + 0.5 * h * k21, y2 + 0.5 * h * k22, y3 + 0.5 * h * k23, y4 + 0.5 * h * k24, y5 + 0.5 * h * k25, prm)
k34 = fff4(x + 0.5 * h, y1 + 0.5 * h * k21, y2 + 0.5 * h * k22, y3 + 0.5 * h * k23, y4 + 0.5 * h * k24, y5 + 0.5 * h * k25, prm)
k35 = fff5(x + 0.5 * h, y1 + 0.5 * h * k21, y2 + 0.5 * h * k22, y3 + 0.5 * h * k23, y4 + 0.5 * h * k24, y5 + 0.5 * h * k25, prm)

```

DHT Example – Visual Basic Model (functions)

```

Public Function fff1(x, y1, y2, y3, y4, y5, prm)
    qs = prm(5) * (prm(6) - prm(2))
    q = qs + prm(4) * (prm(6) - y3) + prm(4) * y4 / prm(8)
    dTdt = (prm(5) * (ti - y1) + q) / prm(1)
    fff2 = (y1 - y2 - (prm(3) / 2) * dTdt) * 2 / prm(3)
End Function

Public Function fff3(x, y1, y2, y3, y4, y5, prm)
    fff3 = (y2 - y3) / prm(7)
End Function

Public Function fff4(x, y1, y2, y3, y4, y5, prm)
    fff4 = prm(6) - y3
End Function

Public Function fff5(x, y1, y2, y3, y4, y5, prm)
    fff5 = 0
End Function

Public Function fff1(x, y1, y2, y3, y4, y5, prm)
    step = 1
    If x < 10 Then
        step = 0
    End If

    ti = prm(2) + step * (-20)

    qs = prm(5) * (prm(6) - prm(2))
    q = qs + prm(4) * (prm(6) - y3) + prm(4) * y4 / prm(8)
    dTdt = (prm(5) * (ti - y1) + q) / prm(1)
    fff1 = dTdt
End Function

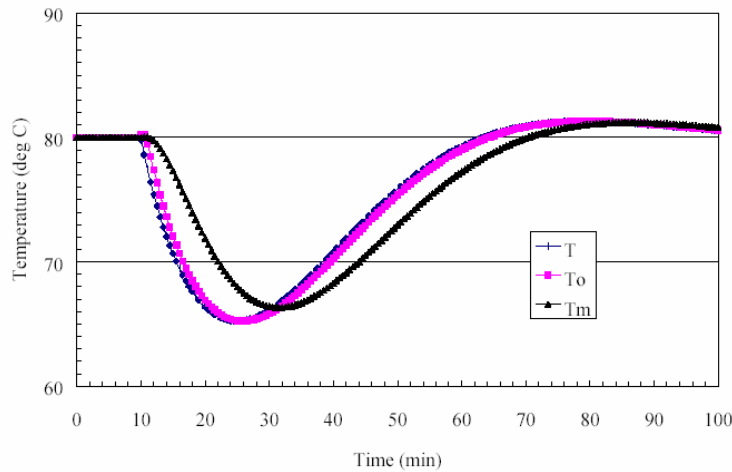
Public Function fff2(x, y1, y2, y3, y4, y5, prm)
    step = 1
    If x < 10 Then
        step = 0
    End If

    ti = prm(2) + step * (-20)

```

Note null function

DHT Example – Excel Solution



Combining the Packages for Greater Efficiency in Effective Problem Solving – POLYMATH and Excel

1. The problem is entered and solved in its basic form using POLYMATH.
2. POLYMATH 6.1 automatically converts the problem into a well documented Excel spreadsheet, ready for solution.
3. The problem can be modified within Excel for parametric studies (using “two input data tables, for example)

DHT Example – Excel Model Generated by POLYMATH

C18 $\❤ = (((C13 - C14) - ((C8 / 2) * (((C5 * (C11 - C13)) + C3) / C6))) * 2) / C8$

	A	B	C	D	E
1	POLYMATH DEQ Migration Document				
2		Variable	Value	Polymath Equation	Comments
3	Explicit Eqs	q	10000	$q=10000+Kc*(Tr-Tm)+Kc/taul*errsum$	Heat supply (k.J)
4		Tr	80	$Tr=80$	Set point tempe.
		WC	500	$WC=500$	(Flow rate)*(hea
		rhoVCp	4000	$rhoVCp=4000$	mass in tank)*(l
		Kc	50	$Kc=50$	Proportional gai
		taud	1	$taud=1$	Dead time (min)
		taum	5	$taum=5$	Thermocouple t
		taul	2	$taul=2$	Reset time (min
		Ti	60	$Ti=60+step$	Feed temperatu
		step	0	$step=if (t < 10) then (0) else (-20)$	Step change in i
13	Integration Vars	T	80	$T(t)=80$	Temperature in
		T0	80	$T(0)=80$	Time delayed te
		Tm	80	$Tm(t)=80$	Temp. measure
		errsum	0	$errsum(0)=0$	Integral of the d
17	ODE Eqs	$d(T)/d(t)$	0	$d(T)/d(t) = (WC*(Ti-T)+q)/rhoVCp$	
		$d(T0)/d(t)$	0	$d(T0)/d(t) = (T-T0-(taud/2)*((WC*(Ti-T)+q)/rhoVCp))*2/taud$	
		$d(Tm)/d(t)$	0	$d(Tm)/d(t) = (T-Tm)/taud$	
		$d(errsum)/d(t)$	0	$d(errsum)/d(t) = T-Tm$	
21	Indep Var	t	0	$t(0)=0 ; t(f)=100$	

POLYMATH converts variable names to cell addresses

Model documentation by variable names, POLYMATH equations and comments

DHT Example – Integrating by the Unique POLYMATH ODE solver for Excel

	A	B	C	D	E
1	POLYMATH DEQ Migration Document				
2		Variable	Value	Polymath Equation	
3	Explicit Eqs	q	20097.27676	$q=10000+Kc*(Tr-Tm)+Kc/taul*errsum$	
4		Tr	80	$Tr=80$	
5		WC	500	$WC=500$	
6		rhoVCp	4000	$rhoVCp=4000$	
7		Kc	50	$Kc=50$	
8		taud	1	$taud=1$	
9		taum	5	$taum=5$	
10		taul	2	$taul=2$	
11		Ti	40	$Ti=60+step$	
12		step	-20	$step=if (t < 10) then (0) else (-20)$	
13	Integration Vars	T	80.5495460	$T(t)=80$	
		T0	80.5943149	$T(0)=80$	
		Tm	80.80866269	$Tm(t)=80$	
		errsum	405.5083959	$errsum(0)=0$	
17	ODE Eqs	$d(T)/d(t)$	-0.044374062	$d(T)/d(t) = (WC*(Ti-T)+q)/rhoVCp$	
		$d(T0)/d(t)$	-0.045524871	$d(T0)/d(t) = (T-T0-(taud/2)*((WC*(Ti-T)+q)/rhoVCp))*2/taud$	
		$d(Tm)/d(t)$	-0.042853441	$d(Tm)/d(t) = (T-Tm)/taud$	
		$d(errsum)/d(t)$	-0.80866269	$d(errsum)/d(t) = T-Tm$	
21	Indep Var	t	100	$t(0)=0 ; t(f)=100$	

Polymath ODE

ODE initial values vector (Y) ODE equations vector (Y')

PL11\$C\$13:\$C\$16 PL11\$C\$17:\$C\$20

Differential variable cell Diffr variable final value

PL11\$C\$21 100

Intermediate cells to Store Data Points

100

Exit Clear Adv. Help Reload Solve

Polymath ODE

Polymath ODE Solver found a solution.

Press OK to keep this solution.

Press Cancel to restore original values.

OK Cancel

DHT Example – MATLAB Model (function)

```
1 function Tdot=tempdyn(t,T)
2 - global qsetpt taud taui Kc Tsetpt onoff
3
4 % Use logical block to model the step change at 10 min.
5 if t<10
6     Tinlet = 60;
7 else
8     Tinlet = 40;
9 end
10
11 qin= qsetpt+Kc*(Tsetpt-T(3))+onoff*Kc/taui*T(4); % total heat sent in
12 row(1)= (500*(Tinlet-T(1))+qin)/4000; % energy balance
13 row(2)= (T(1)-T(2)- 0.5*taud*row(1))/2/taud; % Pade approximation for delay
14 row(3)= (T(2)-T(3))/5; % Thermocouple dynamics
15 row(4)= Tsetpt - T(3); % the integrated error
16
17 Tdot = row;
```

Row(3)=d(Tm)/dt

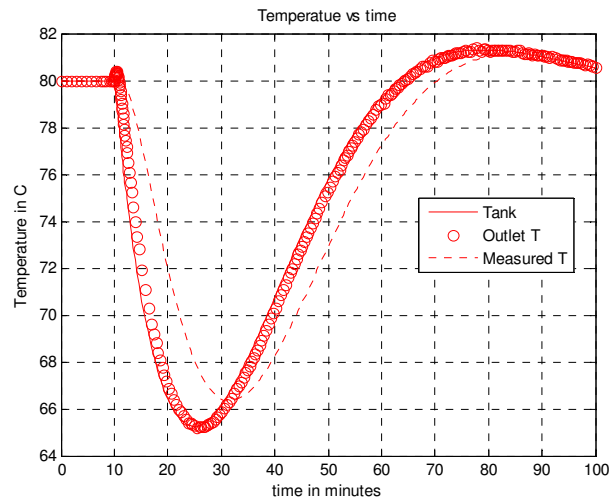
Note the loss of clarity because of the need to define arrays of variables (instead of using variable names) and the special syntax requirements.

DHT Example – MATLAB “Main Program”

```
1 - clear all,clc
2 - global qsetpt taud taui Kc Tsetpt onoff
3 - qsetpt= 1e4; taud=1; taui=2; Tsetpt=80;
4 - Kc= input('enter the gain')
5 - onoff=input('enter 0 for no integrator, enter 1 if integrator on')
6 % initialization
7 - to=0; tf=200; % limits of integration
8 - tspan = [to tf];
9 - To=[80 80 80 0]; % initial condition of system Tank Temp, Outlet Temp
10 % Thermocouple Temp and error signal
11 - [t,T]= ode45('tempdyn',tspan,To);
12 - T
13 - plot(t,T(:,1),r, t,T(:,2),r, t,T(:,3),r);
14 - grid
15 - title('Temperature vs time')
16 - xlabel('time in minutes')
17 - ylabel('Temperature in C')
18 - legend('Tank','Outlet T','Measured T')
```

Note many problem specific components in the “Main Program”

DHT Example – MATLAB Solution



Combining the Packages for Greater Efficiency in Effective Problem Solving – POLYMATH and MATLAB

1. The problem is entered and solved in its basic form using POLYMATH.
2. POLYMATH 6.1 automatically converts the problem into a MATLAB function and provides a template *m* file to run this function.
3. The problem can be modified within MATLAB for parametric studies, optimization, control etc. (using *for* and *while* statements, for example)

DHT Example – MATLAB Model (function) Generated by POLYMATH.

```

1 function dYfuncvecdt = ODEfun(t,Yfuncvec),
2   T = Yfuncvec(1),
3   T0 = Yfuncvec(2),
4   Tm = Yfuncvec(3),
5   errsum = Yfuncvec(4),
6   tauI = 2; %Reset time (min)
7   Tr = 80; %Set point temperature (deg. C)
8   WC = 500; % (Flow rate)/(heat capacity) (kJ/min-deg. C)
9   rhoVCp = 4000; %mass in tank/(heat capacity) (kJ/deg. C)
10  Kc = 50; %Proportional gain of the PI controller (kJ/min-deg. C)
11  taud = 1; %Dead time (min)
12  taum = 5; %Thermocouple time constant (min)
13  q = 10000 + Kc*(Tr - Tm) + Kc/tauI*errsum; %Heat supply (kJ/min)
14  if (t < 10) %Step change in feed temperature (deg. C)
15      step = 0;
16  else
17      step = -20;
18  end
19  T1 = 60 + step; %Feed temperature (deg. C)
20  dTdt = (WC*(T1 - T) + q)/rhoVCp; %Temperature in the stirred tank (deg. C)
21  dT0dt = (T - T0 - (taud/2)*(WC*(T1 - T) + q)/rhoVCp)*2/taud; %Time delayed t
22  dTmtdt = (T0 - Tm)/taum; %Temp. measured by the thermocouple (deg. C)
23  derrsumdt = Tr - Tm; %Integral of the difference between set point and
24  dYfuncvecdt = [dTdt; dT0dt; dTmtdt; derrsumdt];

```

Note consistent use of variable names and reordering the equations

DHT Example – MATLAB “Main Program” Available in the POLYMATH “Help”

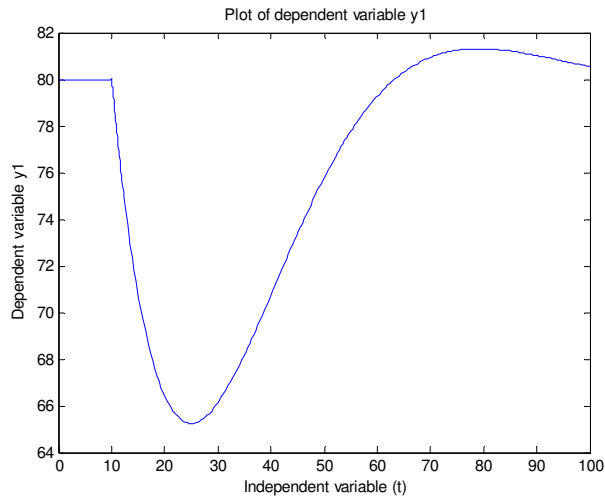
```

1 function Prob_10
2 clear, clc, format short g, format compact
3 tspan = [0 100.]; % Range for the independent variable
4 y0 = [80; 80; 80; 0]; % Initial values for the dependent variables
5 disp('Variable values at the initial point ');
6 disp([' t = ' num2str(tspan(1))]);
7 disp([' y dy/dt ']);
8 disp([y0 ODEfun(tspan(1),y0)]);
9 [t,y]=ode45(@ODEfun,tspan,y0);
10 for i=1:size(y,2)
11     disp([' Solution for dependent variable y' int2str(i)]);
12     disp([' t y' int2str(i)]);
13     disp([t y(i)]);
14     plot(t,y(i));
15     title([' Plot of dependent variable y' int2str(i)]);
16     xlabel(' Independent variable (t)');
17     ylabel([' Dependent variable y' int2str(i)]);
18     pause
19 end

```

Only the initial and final values are problem specific

DHT Example – MATLAB Solution Using the Program Generated by POLYMATH



Conclusions

The Excel worksheets and MATLAB functions generated by POLYMATH are *well documented problem models of uniform structure* obtained by minimal effort on behalf of the user.

These models can be easily modified to carry out *parametric studies, optimization, control*, etc., automatically. Thus the advantages of the various programs can be fully utilized while the required effort is reduced.

The POLYMATH conversion utility provides also considerable *educational benefits* by enabling learning of Excel and MATLAB by modifying existing spreadsheets or programs. *Learning by modification* may prevent frustration caused by repeated failures to obtain a working program when programming from scratch.

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